



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 12:32 am GMT

PDB ID : 5CYY  
Title : Structure of the C-terminal domains of DipZ from Mycobacterium tuberculosis  
Authors : Goldstone, D.C.; Metcalf, P.; Baker, E.N.; Mycobacterium Tuberculosis Structural Proteomics Project (XMTB)  
Deposited on : 2015-07-31  
Resolution : 2.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

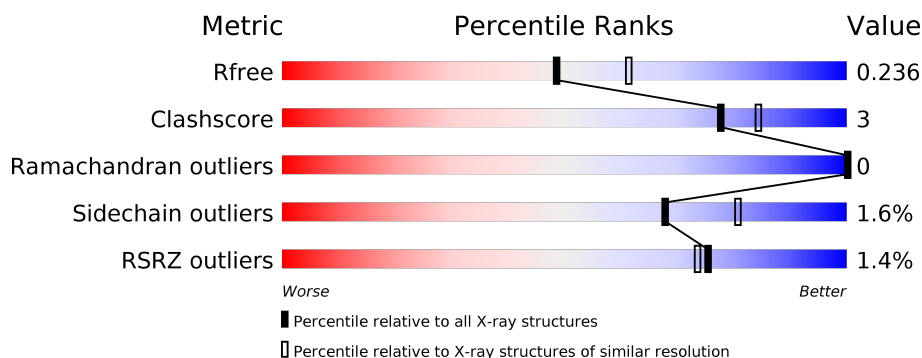
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	360	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 85%, green 85%, grey 85%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>85%</span> <span>8%</span> <span>8%</span> </div> </div>
1	B	360	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 3%, yellow 82%, green 82%, grey 82%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>82%</span> <span>9%</span> <span>9%</span> </div> </div>
1	C	360	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 84%, green 84%, grey 84%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>84%</span> <span>9%</span> <span>8%</span> </div> </div>
1	D	360	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 83%, green 83%, grey 83%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>83%</span> <span>8%</span> <span>8%</span> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10471 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Protein DipZ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	0	0
			2511	1597	425	485	4			
1	B	328	Total	C	N	O	S	0	0	0
			2456	1562	414	476	4			
1	C	333	Total	C	N	O	S	0	2	0
			2520	1600	430	484	6			
1	D	331	Total	C	N	O	S	0	2	0
			2498	1588	426	478	6			

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	336	MET	-	initiating methionine	UNP P9WG63
A	337	SER	-	expression tag	UNP P9WG63
A	338	TYR	-	expression tag	UNP P9WG63
A	339	TYR	-	expression tag	UNP P9WG63
A	340	HIS	-	expression tag	UNP P9WG63
A	341	HIS	-	expression tag	UNP P9WG63
A	342	HIS	-	expression tag	UNP P9WG63
A	343	HIS	-	expression tag	UNP P9WG63
A	344	HIS	-	expression tag	UNP P9WG63
A	345	HIS	-	expression tag	UNP P9WG63
A	346	ASP	-	expression tag	UNP P9WG63
A	347	TYR	-	expression tag	UNP P9WG63
A	348	ASP	-	expression tag	UNP P9WG63
A	349	ILE	-	expression tag	UNP P9WG63
A	350	PRO	-	expression tag	UNP P9WG63
A	351	THR	-	expression tag	UNP P9WG63
A	352	THR	-	expression tag	UNP P9WG63
A	353	GLU	-	expression tag	UNP P9WG63
A	354	ASN	-	expression tag	UNP P9WG63
A	355	LEU	-	expression tag	UNP P9WG63
A	356	TYR	-	expression tag	UNP P9WG63

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Chain	Residue	Modelled	Actual	Comment	Reference
A	357	PHE	-	expression tag	UNP P9WG63
A	358	GLN	-	expression tag	UNP P9WG63
A	359	GLY	-	expression tag	UNP P9WG63
A	360	ALA	-	expression tag	UNP P9WG63
B	336	MET	-	initiating methionine	UNP P9WG63
B	337	SER	-	expression tag	UNP P9WG63
B	338	TYR	-	expression tag	UNP P9WG63
B	339	TYR	-	expression tag	UNP P9WG63
B	340	HIS	-	expression tag	UNP P9WG63
B	341	HIS	-	expression tag	UNP P9WG63
B	342	HIS	-	expression tag	UNP P9WG63
B	343	HIS	-	expression tag	UNP P9WG63
B	344	HIS	-	expression tag	UNP P9WG63
B	345	HIS	-	expression tag	UNP P9WG63
B	346	ASP	-	expression tag	UNP P9WG63
B	347	TYR	-	expression tag	UNP P9WG63
B	348	ASP	-	expression tag	UNP P9WG63
B	349	ILE	-	expression tag	UNP P9WG63
B	350	PRO	-	expression tag	UNP P9WG63
B	351	THR	-	expression tag	UNP P9WG63
B	352	THR	-	expression tag	UNP P9WG63
B	353	GLU	-	expression tag	UNP P9WG63
B	354	ASN	-	expression tag	UNP P9WG63
B	355	LEU	-	expression tag	UNP P9WG63
B	356	TYR	-	expression tag	UNP P9WG63
B	357	PHE	-	expression tag	UNP P9WG63
B	358	GLN	-	expression tag	UNP P9WG63
B	359	GLY	-	expression tag	UNP P9WG63
B	360	ALA	-	expression tag	UNP P9WG63
C	336	MET	-	initiating methionine	UNP P9WG63
C	337	SER	-	expression tag	UNP P9WG63
C	338	TYR	-	expression tag	UNP P9WG63
C	339	TYR	-	expression tag	UNP P9WG63
C	340	HIS	-	expression tag	UNP P9WG63
C	341	HIS	-	expression tag	UNP P9WG63
C	342	HIS	-	expression tag	UNP P9WG63
C	343	HIS	-	expression tag	UNP P9WG63
C	344	HIS	-	expression tag	UNP P9WG63
C	345	HIS	-	expression tag	UNP P9WG63
C	346	ASP	-	expression tag	UNP P9WG63
C	347	TYR	-	expression tag	UNP P9WG63
C	348	ASP	-	expression tag	UNP P9WG63

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Chain	Residue	Modelled	Actual	Comment	Reference
C	349	ILE	-	expression tag	UNP P9WG63
C	350	PRO	-	expression tag	UNP P9WG63
C	351	THR	-	expression tag	UNP P9WG63
C	352	THR	-	expression tag	UNP P9WG63
C	353	GLU	-	expression tag	UNP P9WG63
C	354	ASN	-	expression tag	UNP P9WG63
C	355	LEU	-	expression tag	UNP P9WG63
C	356	TYR	-	expression tag	UNP P9WG63
C	357	PHE	-	expression tag	UNP P9WG63
C	358	GLN	-	expression tag	UNP P9WG63
C	359	GLY	-	expression tag	UNP P9WG63
C	360	ALA	-	expression tag	UNP P9WG63
D	336	MET	-	initiating methionine	UNP P9WG63
D	337	SER	-	expression tag	UNP P9WG63
D	338	TYR	-	expression tag	UNP P9WG63
D	339	TYR	-	expression tag	UNP P9WG63
D	340	HIS	-	expression tag	UNP P9WG63
D	341	HIS	-	expression tag	UNP P9WG63
D	342	HIS	-	expression tag	UNP P9WG63
D	343	HIS	-	expression tag	UNP P9WG63
D	344	HIS	-	expression tag	UNP P9WG63
D	345	HIS	-	expression tag	UNP P9WG63
D	346	ASP	-	expression tag	UNP P9WG63
D	347	TYR	-	expression tag	UNP P9WG63
D	348	ASP	-	expression tag	UNP P9WG63
D	349	ILE	-	expression tag	UNP P9WG63
D	350	PRO	-	expression tag	UNP P9WG63
D	351	THR	-	expression tag	UNP P9WG63
D	352	THR	-	expression tag	UNP P9WG63
D	353	GLU	-	expression tag	UNP P9WG63
D	354	ASN	-	expression tag	UNP P9WG63
D	355	LEU	-	expression tag	UNP P9WG63
D	356	TYR	-	expression tag	UNP P9WG63
D	357	PHE	-	expression tag	UNP P9WG63
D	358	GLN	-	expression tag	UNP P9WG63
D	359	GLY	-	expression tag	UNP P9WG63
D	360	ALA	-	expression tag	UNP P9WG63

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	135	Total O 135 135	0	0

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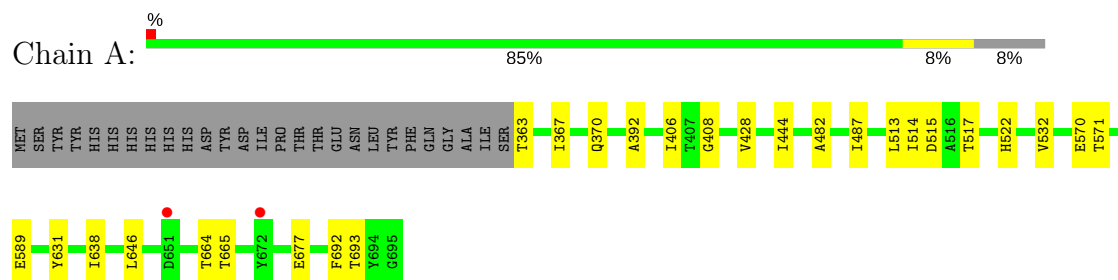
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	91	Total 91	O 91	0	0
2	C	130	Total 130	O 130	0	0
2	D	130	Total 130	O 130	0	0

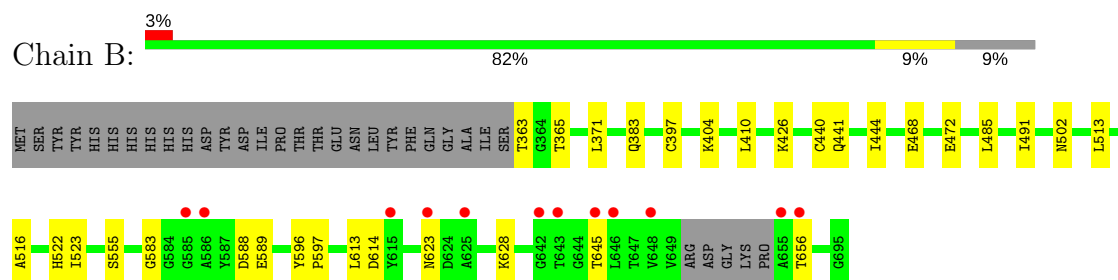
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

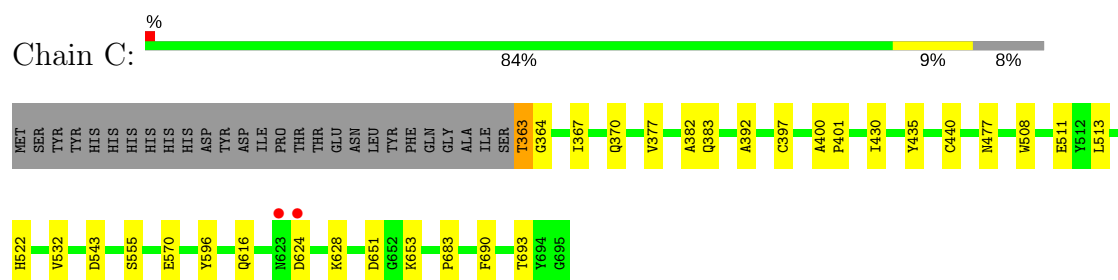
#### • Molecule 1: Protein DipZ



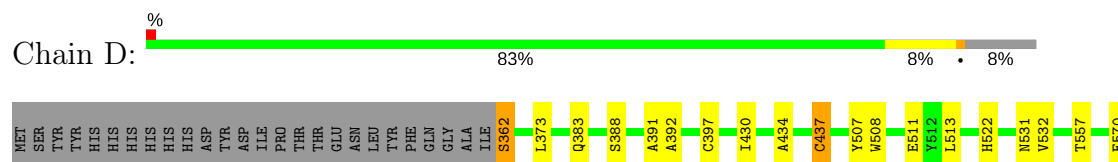
#### • Molecule 1: Protein DipZ



#### • Molecule 1: Protein DipZ



#### • Molecule 1: Protein DipZ







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.97Å 117.53Å 122.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.39 – 2.20 42.39 – 2.20	Depositor EDS
% Data completeness (in resolution range)	90.1 (42.39-2.20) 90.2 (42.39-2.20)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.77 (at 2.20Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.182 , 0.237 0.183 , 0.236	Depositor DCC
$R_{free}$ test set	7296 reflections (9.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.0	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 34.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.035 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10471	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.17% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.40	0/2575	0.54	0/3522
1	B	0.37	0/2517	0.54	0/3445
1	C	0.42	0/2589	0.55	0/3538
1	D	0.41	0/2566	0.56	0/3507
All	All	0.40	0/10247	0.55	0/14012

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2511	0	2433	15	0
1	B	2456	0	2366	15	0
1	C	2520	0	2459	18	0
1	D	2498	0	2435	21	0
2	A	135	0	0	3	0
2	B	91	0	0	2	0
2	C	130	0	0	2	0
2	D	130	0	0	4	0
All	All	10471	0	9693	66	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 66 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:THR:N	2:A:704:HOH:O	2.30	0.64
1:B:363:THR:N	2:B:701:HOH:O	2.32	0.62
1:D:610:ARG:HG2	1:D:621:ASP:HB3	1.82	0.61
1:C:570:GLU:HG3	1:C:693:THR:HG22	1.85	0.59
1:C:651:ASP:HB2	1:C:653:LYS:HE2	1.84	0.58

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	331/360 (92%)	321 (97%)	10 (3%)	0	100	100
1	B	324/360 (90%)	311 (96%)	13 (4%)	0	100	100
1	C	333/360 (92%)	325 (98%)	8 (2%)	0	100	100
1	D	329/360 (91%)	310 (94%)	19 (6%)	0	100	100
All	All	1317/1440 (92%)	1267 (96%)	50 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	259/288 (90%)	258 (100%)	1 (0%)	93	97
1	B	252/288 (88%)	247 (98%)	5 (2%)	60	74
1	C	263/288 (91%)	260 (99%)	3 (1%)	78	88
1	D	260/288 (90%)	252 (97%)	8 (3%)	45	57
All	All	1034/1152 (90%)	1017 (98%)	17 (2%)	68	81

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	624	ASP
1	C	683	PRO
1	D	599	SER
1	C	363	THR
1	D	608	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	333/360 (92%)	-0.42	2 (0%) 89 88	20, 31, 50, 65	0
1	B	328/360 (91%)	-0.10	12 (3%) 42 40	22, 36, 66, 79	0
1	C	333/360 (92%)	-0.40	2 (0%) 89 88	20, 29, 46, 73	0
1	D	331/360 (91%)	-0.34	3 (0%) 84 83	21, 32, 48, 71	0
All	All	1325/1440 (92%)	-0.32	19 (1%) 75 73	20, 32, 58, 79	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	586	ALA	6.0
1	C	624	ASP	4.2
1	B	615	TYR	3.8
1	C	623	ASN	3.1
1	B	585	GLY	3.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.